

Methyl (pentyloxy)acetate
70081-24-2 | DTXSID30220355

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.64e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.18e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Nonanoic acid</div> <div>Measured: 3.75e-01</div> <div>Predicted: 1.91e-03</div>	<div>Image not found</div> <div>Heptanoic acid</div> <div>Measured: 2.34</div> <div>Predicted: 6.20e-03</div>	<div>Image not found</div> <div>2-Butanamine</div> <div>Measured: 1.02e-01</div> <div>Predicted: 179</div>
<div>Image not found</div> <div>Formamide, N-(1,1-dimethylethyl)-</div> <div>Measured: 3.20</div> <div>Predicted: 3.16e-01</div>	<div>Image not found</div> <div>bis(2-Chloro-1-methylethyl) ether</div> <div>Measured: 3.92</div> <div>Predicted: 1.62</div>	